

# Sharply Bounding the Holevo Quantity

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## Abstract

For a quantum ensemble  $\mathcal{E}_3 = \{(p_i, \rho_i)\}_{i=1}^3$ , M. Fannes *et al.* conjectured that the entropy of the correlation matrix of  $\mathcal{E}_3 = \{(p_i, \rho_i)\}_{i=1}^3$  is upper bound for the Holevo quantity  $\chi(\mathcal{E}_3)$  of quantum ensemble  $\mathcal{E}_3 = \{(p_i, \rho_i)\}_{i=1}^3$ . In this paper, we prove the conjecture under a strictly constraint condition.

## 1 Introduction and preliminaries

Let  $\mathcal{H}^1$  be a finite dimensional complex Hilbert space. A *quantum state*  $\rho$  on  $\mathcal{H}^1$  is a positive semi-definite operator of trace one, in particular, for each unit vector  $|\psi\rangle \in \mathcal{H}^1$ , the operator  $\rho = |\psi\rangle\langle\psi|$  is said to be a pure state. The set of all states on  $\mathcal{H}^1$  is denoted by  $D(\mathcal{H})$ . For each quantum state  $\rho \in D(\mathcal{H})$ , its von Neumann entropy is defined by  $S(\rho) = -\text{Tr}(\rho \log \rho)$ . If  $\rho$  and  $\sigma$  are two states on  $\mathcal{H}^1$ , then  $F(\rho, \sigma) = \text{Tr}(|\sqrt{\rho}\sqrt{\sigma}|)^2$  is said to be the *fidelity* between  $\rho$  and  $\sigma$ . A *quantum operation*  $\Phi$  on  $\mathcal{H}^1$  is a completely positive linear mapping defined on the set  $D(\mathcal{H}^1)$ . It follows from ([1], Prop. 5.2 and Coro. 5.5) that there exists linear operators  $\{M_\mu\}_{\mu=1}^K$  on  $\mathcal{H}^1$  such that  $\sum_{\mu=1}^K M_\mu^\dagger M_\mu = \mathbb{1}^1$  and for each quantum state  $\rho$ , we have the Kraus representation

$$\Phi(\rho) = \sum_{\mu=1}^K M_\mu \rho M_\mu^\dagger.$$

Moreover, let  $\mathcal{H}^2 = \mathbb{C}^K$  and  $\{|\mu\rangle\}_{\mu=1}^K$  be the standard orthonormal basis of  $\mathcal{H}^2$ . A quantum operation  $\hat{\Phi}$  from the system  $\mathcal{H}^1$  to the system  $\mathcal{H}^2$  is called *complementary* to  $\Phi$  if

$$\hat{\Phi} : \rho \mapsto \hat{\Phi}(\rho) = \sum_{\mu, \nu} \text{Tr}(M_\mu \rho M_\nu^\dagger) |\mu\rangle\langle\nu|, \quad (1.1)$$

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the state  $\widehat{\Phi}(\rho)$  on  $\mathcal{H}^2$  describes the correlation between  $\mathcal{H}^1$  and  $\mathcal{H}^2$ .

Note that  $\sum_{\mu=1}^K M_{\mu}^{\dagger} M_{\mu} = \mathbb{1}^1$ , so  $\{M_{\mu}\}_{\mu=1}^K$  decides a quantum measurement which transforms an initial state  $\rho$  into one of the output states

$$\rho'_{\mu} = \frac{1}{q_{\mu}} M_{\mu} \rho M_{\mu}^{\dagger}$$

with probability  $q_{\mu} = \text{Tr} (M_{\mu} \rho M_{\mu}^{\dagger})$ , where  $\mu = 1, 2, \dots, K$ . The *Holevo quantity* of the quantum ensemble  $\{(q_{\mu}, \rho'_{\mu})\}$  is defined by the following expression:

$$\chi \{(q_{\mu}, \rho'_{\mu})\} = S \left( \sum_{\mu} q_{\mu} \rho'_{\mu} \right) - \sum_{\mu} q_{\mu} S (\rho'_{\mu}). \quad (1.2)$$

In [2], the following important inequality was obtained:

$$\chi \{(q_{\mu}, \rho'_{\mu})\} \leq S (\widehat{\Phi}(\rho)) \leq H (\{q_{\mu}\}), \quad (1.3)$$

where  $H (\{q_{\mu}\}) = -\sum_{\mu} q_{\mu} \log q_{\mu}$  is the Shannon entropy of a probability distribution  $\{q_{\mu}\}$ .

Let  $\mathcal{E}_K = \{(p_i, \rho_i)\}_{i=1}^K$  be a quantum ensemble on  $\mathcal{H}^1$ , that is, each  $\rho_i \in \mathcal{D}(\mathcal{H}^1)$ ,  $p_i > 0$ , and  $\sum_{i=1}^K p_i = 1$ . The matrix

$$C_{\sqrt{F}}(\mathcal{E}_K) = \left( \sqrt{p_i p_j F_{ij}} \right)_{ij}$$

is said to be a *correlation matrix* of the quantum ensemble  $\mathcal{E}_K = \{(p_i, \rho_i)\}_{i=1}^K$ , where  $F_{ij} = F(\rho_i, \rho_j)$  is the fidelity between  $\rho_i$  and  $\rho_j$ .

For  $K = 2$  or  $3$ , the correlation matrix  $C_{\sqrt{F}}(\mathcal{E}_K) = (\sqrt{p_i p_j F_{ij}})_{ij}$  is a legitimate state accordingly, however, if  $K \geq 4$ , then  $C_{\sqrt{F}}(\mathcal{E}_K) = (\sqrt{p_i p_j F_{ij}})_{ij}$  fails to be positive in general [3]. For  $K = 2$ , the correlation matrix

$$\begin{pmatrix} p_1 & \sqrt{p_1 p_2 F(\rho_1, \rho_2)} \\ \sqrt{p_1 p_2 F(\rho_1, \rho_2)} & p_2 \end{pmatrix}.$$

was shown to satisfy the following inequality [2]:

$$\chi(\mathcal{E}_2) \leq S \left( \begin{pmatrix} p_1 & \sqrt{p_1 p_2 F(\rho_1, \rho_2)} \\ \sqrt{p_1 p_2 F(\rho_1, \rho_2)} & p_2 \end{pmatrix} \right).$$

Motivated by the above fact, M. Fannes *et al.* proposed the following conjecture in [3]:

**Conjecture:** For  $K = 3$ ,  $\chi(\mathcal{E}_3) \leq S(C_{\sqrt{F}}(\mathcal{E}_3))$  is also true.

In this paper, we prove the conjecture under some constraint condition.

## 2 Technical lemmas

Let  $\mathcal{H}^A$  and  $\mathcal{H}^B$  be two finite dimensional complex Hilbert spaces,  $\rho^{AB}$  is a state on  $\mathcal{H}^A \otimes \mathcal{H}^B$ ,  $\rho^A = \text{Tr}_B(\rho^{AB})$ ,  $\rho^B = \text{Tr}_A(\rho^{AB})$ .

$$\Pi^B(\rho^{AB}) = \sum_j (\mathbb{1}^A \otimes \Pi_j^B) \rho^{AB} (\mathbb{1}^A \otimes \Pi_j^B)$$

is the output state after executing the nonselective measurement  $\Pi^B = \{\Pi_j^B\}$ ;  $\mathbb{1}^A$  is the identity operator on  $\mathcal{H}^A$ .

Let  $\{|\psi_j^B\rangle\}_{j=1}^k$  be a orthonormal basis of  $\mathcal{H}^B$  and  $\Pi_j^B = |\psi_j^B\rangle\langle\psi_j^B|$ . Then

$$\text{Tr}(\mathbb{1}^A \otimes \Pi_j^B \rho^{AB} \mathbb{1}^A \otimes \Pi_j^B) = \langle\psi_j^B|\rho^B|\psi_j^B\rangle.$$

If we denote  $\langle\psi_j^B|\rho^B|\psi_j^B\rangle$  by  $p_j$ , then  $p_j \geq 0$  and  $\sum_j p_j = 1$ . Without loss of generality, we assume that all  $p_j > 0$ . Now, we define  $\rho_j^A = \langle\psi_j^B|\rho^{AB}|\psi_j^B\rangle/p_j$ , then  $\rho_j^A$  is a state on  $\mathcal{H}^A$  and

$$\Pi^B(\rho^{AB}) = \sum_j p_j \rho_j^A \otimes \Pi_j^B, \quad \Pi^B(\rho^B) = \sum_j p_j \Pi_j^B, \quad \rho^A = \sum_j p_j \rho_j^A.$$

The following result appeared in the proof in [4], in order to be convenient for our presentation, we reformulate it as a separate result. Furthermore, we will generalize it to the case where von Neumann measurements are replaced by general POVMs.

**Lemma 2.1.** *If the von Neumann measurement performed on the subsystem B induces an ensemble  $\mathcal{E}_K = \{(p_j, \rho_j^A)\}$  on the subsystem A, then*

$$\chi\left\{(p_j, \rho_j^A)\right\} \leq S(\rho^B), \quad (2.1)$$

where  $K = \dim(\mathcal{H}^B)$ .

*Proof.* Note that the quantum ensemble  $\{(p_j, \rho_j^A)\}$  is obtained from the quantum operation of taking partial trace over  $\mathcal{H}^B$  from the quantum state  $\rho^{AB}$ , this inspired us to define the following quantum operation  $\Psi$  on the quantum system  $\mathcal{H}^A \otimes \mathcal{H}^B$ :

Let  $|\omega^B\rangle \in \mathcal{H}^B$  be a fixed unit vector, for each quantum state  $\sigma^{AB}$  on  $\mathcal{H}^A \otimes \mathcal{H}^B$ ,

$$\begin{aligned} \Psi(\sigma^{AB}) &= \sum_j (\mathbb{1}^A \otimes |\omega^B\rangle\langle\psi_j^B|) \sigma^{AB} (\mathbb{1}^A \otimes |\omega^B\rangle\langle\psi_j^B|)^\dagger \\ &= \text{Tr}_B(\sigma^{AB}) \otimes |\omega^B\rangle\langle\omega^B|. \end{aligned}$$

Let  $\mathcal{H}^C = \mathbb{C}^k$  and  $\{|i\rangle\}_{i=1}^k$  be the standard orthonormal basis of  $\mathcal{H}^C$ . Then the correlation matrix  $\hat{\Psi}(\rho^{AB})$  is given by

$$\begin{aligned}\hat{\Psi}(\rho^{AB}) &= \sum_{i,j} \text{Tr} \left( \left( \mathbb{1}^A \otimes |\omega^B\rangle\langle\psi_i^B| \right) \rho^{AB} \left( \mathbb{1}^A \otimes |\psi_j^B\rangle\langle\omega^B| \right) \right) |i\rangle\langle j| \\ &= \sum_{i,j} \langle \psi_i^B | \rho^B | \psi_j^B \rangle |i\rangle\langle j|,\end{aligned}$$

If we define  $W = \sum_j |j\rangle\langle\psi_j^B|$ , then  $W^\dagger W = \mathbb{1}^B$ ,  $WW^\dagger = \mathbb{1}^C$ , that is,  $W$  is a unitary operator from  $\mathcal{H}^B$  to  $\mathcal{H}^C$ . It follows from  $\hat{\Psi}(\rho^{AB}) = W\rho^B W^\dagger$  that  $S(\hat{\Psi}(\rho^{AB})) = S(\rho^B)$ . Note that the quantum ensemble  $\left\{ (p_j, \rho_j^A \otimes |\omega^B\rangle\langle\omega^B|) \right\}$  can be obtained by the quantum operation  $\Psi$  and  $\chi \left\{ (p_j, \rho_j^A) \right\} = \chi \left\{ (p_j, \rho_j^A \otimes |\omega^B\rangle\langle\omega^B|) \right\}$ . By using the inequality (1.3) we have

$$\chi \left\{ (p_j, \rho_j^A) \right\} = \chi \left\{ (p_j, \rho_j^A \otimes |\omega^B\rangle\langle\omega^B|) \right\} \leq S(\hat{\Psi}(\rho^{AB})) = S(\rho^B).$$

□

In what follows, we generalize the above inequality (2.1) to the case where the von Neumann measurement is replaced by POVMs. Firstly, we generalize it to PVM case.

Let  $\rho^{AB} \in \mathcal{D}(\mathcal{H}^A \otimes \mathcal{H}^B)$  and  $P^B$  is a projection on  $\mathcal{H}^B$ . For the projection  $P^B$ , there exists an orthonormal set  $\{|u_i\rangle : i = 1, \dots, m \leq \dim(\mathcal{H}^B)\}$  of vectors in  $\mathcal{H}^B$  such that  $P^B = \sum_{i=1}^m |u_i\rangle\langle u_i|$ . Denote  $\tilde{p} = \text{Tr}(\mathbb{1}^A \otimes P^B \rho^{AB} \mathbb{1}^A \otimes P^B)$  and  $\tilde{\rho}^A = \text{Tr}_B(\mathbb{1}^A \otimes P^B \rho^{AB} \mathbb{1}^A \otimes P^B)$ ,  $p_i \rho_i^A = \langle u_i | \rho^{AB} | u_i \rangle$ , where  $p_i = \langle u_i | \rho^B | u_i \rangle$ ,  $\rho^B = \text{Tr}_A(\rho^{AB})$ . Then we have the following proposition:

**Proposition 2.2.**  $\tilde{p} S(\tilde{\rho}^A) \geq \sum_{i=1}^m p_i S(\rho_i^A)$ .

*Proof.* In fact,

$$\begin{aligned}\tilde{p} &= \text{Tr}(\mathbb{1}^A \otimes P^B \rho^{AB} \mathbb{1}^A \otimes P^B) = \text{Tr}(\mathbb{1}^A \otimes P^B \rho^{AB}) \\ &= \sum_{i=1}^m \text{Tr}(\langle u_i | \rho^{AB} | u_i \rangle) = \sum_{i=1}^m \langle u_i | \rho^B | u_i \rangle = \sum_{i=1}^m p_i,\end{aligned}$$

and  $\mathbb{1}^A \otimes P^B \rho^{AB} \mathbb{1}^A \otimes P^B = \sum_{i,i'=1}^m \langle u_i | \rho^{AB} | u_{i'} \rangle \otimes |u_i\rangle\langle u_{i'}|$ , which implies that

$$\tilde{p} \tilde{\rho}^A = \sum_{i=1}^m p_i \rho_i^A.$$

Now the desired inequality follows from the concavity of von Neumann entropy. □

Given a PVM  $\{P_\mu^B\}$  on the subsystem  $B$ , there corresponds an orthonormal basis  $\{|\phi_j\rangle : j = 1, \dots, \dim(\mathcal{H}^B)\}$  for which each  $P_\mu^B$  is a sum of some rank-one projectors  $|\phi_j\rangle\langle\phi_j|$  and we have  $\tilde{p}_\mu \tilde{\rho}_\mu^A = \text{Tr}_B \left( \mathbb{1}^A \otimes P_\mu^B \rho^{AB} \mathbb{1}^A \otimes P_\mu^B \right)$ , where  $\tilde{p}_\mu = \text{Tr} \left( \mathbb{1}^A \otimes P_\mu^B \rho^{AB} \mathbb{1}^A \otimes P_\mu^B \right)$ . Similarly,  $p_j \rho_j^A = \langle\phi_j| \rho^{AB} |\phi_j\rangle$ , where  $p_j = \langle\phi_j| \rho^B |\phi_j\rangle$ ,  $\rho^B = \text{Tr}_A(\rho^{AB})$ . Now we can state our first generalization:

**Proposition 2.3.** *With the above notation, we have*

$$\chi \left\{ \left( \tilde{p}_\mu, \tilde{\rho}_\mu^A \right) \right\} \leq \chi \left\{ \left( p_j, \rho_j^A \right) \right\}.$$

*Proof.* Since each index set  $\{\mu\}$  determine a partition of the set  $\{1, \dots, \dim(\mathcal{H}^B)\}$ :

$$\{1, \dots, \dim(\mathcal{H}^B)\} = \bigcup_{\mu} \Gamma_\mu,$$

where  $\Gamma_\mu \cap \Gamma_{\mu'} = \emptyset$  if  $\mu \neq \mu'$ . Thus it follows from Proposition 2.2 that

$$\tilde{p}_\mu S \left( \tilde{\rho}_\mu^A \right) \geq \sum_{j \in \Gamma_\mu} p_j S \left( \rho_j^A \right), \quad \forall \mu.$$

This indicates that

$$\sum_{\mu} \tilde{p}_\mu S \left( \tilde{\rho}_\mu^A \right) \geq \sum_{\mu} \sum_{j \in \Gamma_\mu} p_j S \left( \rho_j^A \right) = \sum_j p_j S \left( \rho_j^A \right),$$

which gives the desired result.  $\square$

In order to obtain a general POVM case, we employ the Naimark's theorem:

**Theorem 2.4.** (Naimark's Theorem). *Let  $\{E_\mu\}$  be a POVM on a Hilbert space  $\mathcal{H}$ . Then there exist a Hilbert space  $\mathcal{K}$  and a linear isometry  $V$  on  $\mathcal{H} \otimes \mathcal{K}$  such that*

$$E_\mu = V^\dagger (\mathbb{1}_{\mathcal{H}} \otimes |\mu\rangle\langle\mu|) V$$

for all  $\mu$ .

Now for any fixed choice of a normalized vector  $|\varepsilon\rangle \in \mathcal{K}$ , we can choose a unitary operator  $U$  on  $\mathcal{H} \otimes \mathcal{K}$  such that  $V = U(\mathbb{1}_{\mathcal{H}} \otimes |\varepsilon\rangle)$ . Consider a PVM  $\{\Pi_\mu\}$  which is defined by

$$\Pi_\mu = U^\dagger (\mathbb{1}_{\mathcal{H}} \otimes |\mu\rangle\langle\mu|) U$$

for all  $\mu$ . It is easily seen that

$$\text{Tr} (\Pi_\mu (\rho \otimes |\varepsilon\rangle\langle\varepsilon|)) = \text{Tr} (E_\mu \rho), \quad \langle\varepsilon| \Pi_\mu |\varepsilon\rangle = E_\mu.$$

Now we can state our the more general result as follows: Given a POVM  $\{E_\mu^B\}$  on the subsystem  $B$ , we have  $\tilde{p}_\mu \tilde{\rho}_\mu^A = \text{Tr}_B \left( \mathbb{1}^A \otimes \sqrt{E_\mu^B} \rho^{AB} \mathbb{1}^A \otimes \sqrt{E_\mu^B} \right)$ , where  $\tilde{p}_\mu = \text{Tr} \left( \mathbb{1}^A \otimes \sqrt{E_\mu^B} \rho^{AB} \mathbb{1}^A \otimes \sqrt{E_\mu^B} \right)$ . By Naimark's Theorem 2.4, there exist an ancillary system  $C$  and a fixed normalized vector  $|0\rangle^C$ , a PVM  $\{\Pi_\mu^{BC}\}$  on the composite system  $BC$  such that  $\langle 0 | \Pi_\mu^{BC} | 0 \rangle = E_\mu^B$ .

$$\tilde{p}_\mu \tilde{\rho}_\mu^A = \text{Tr}_B \left( \mathbb{1}^A \otimes \sqrt{E_\mu^B} \rho^{AB} \mathbb{1}^A \otimes \sqrt{E_\mu^B} \right) = \text{Tr}_{BC} \left( \mathbb{1}^A \otimes \Pi_\mu^{BC} \rho^{AB} \otimes |0\rangle\langle 0|^C \mathbb{1}^A \otimes \Pi_\mu^{BC} \right),$$

which, together with Lemma 2.1 and Proposition 2.3, implies that

$$\chi \left\{ \left( \tilde{p}_\mu, \tilde{\rho}_\mu^A \right) \right\} \leq S \left( \rho^B \otimes |0\rangle\langle 0|^C \right) = S \left( \rho^B \right).$$

Given a quantum operation  $\Phi^B$  on subsystem  $B$ , it follows from Choi-Kraus representation Theorem that there is a collection of Kraus operators

$$\left\{ M_\mu^B : \mu = 1, \dots, K \leq \left( \dim \left( \mathcal{H}^B \right) \right)^2 \right\}$$

such that  $\Phi^B = \sum_\mu \mathbf{A} \mathbf{d}_{M_\mu^B}$ . The trace-preservation of  $\Phi^B$  means that  $\sum_\mu M_\mu^{B\dagger} M_\mu^B = \mathbb{1}^B$ , which implies that  $\{M_\mu^{B\dagger} M_\mu^B\}$  is a legitimate POVM. Now the measurement statistics of  $\Phi^B$  may be simulated by the POVM  $\{M_\mu^{B\dagger} M_\mu^B\}$  as follows:

$$\begin{aligned} \tilde{p}_\mu \tilde{\rho}_\mu^A &= \text{Tr}_B \left( \left( \mathbb{1}^A \otimes M_\mu^B \right) \rho^{AB} \left( \mathbb{1}^A \otimes M_\mu^B \right)^\dagger \right) \\ &= \text{Tr}_B \left( \left( \mathbb{1}^A \otimes M_\mu^{B\dagger} M_\mu^B \right) \rho^{AB} \right) \\ &= \text{Tr}_B \left( \left( \mathbb{1}^A \otimes \sqrt{M_\mu^{B\dagger} M_\mu^B} \right) \rho^{AB} \left( \mathbb{1}^A \otimes \sqrt{M_\mu^{B\dagger} M_\mu^B} \right) \right). \end{aligned}$$

It is easily seen that the quantum operation  $\Phi^B$  induced a quantum ensemble  $\left\{ \left( \tilde{p}_\mu, \tilde{\rho}_\mu^A \right) \right\}$  on subsystem  $A$ , it follows from the above discussion that

$$\chi \left\{ \left( \tilde{p}_\mu, \tilde{\rho}_\mu^A \right) \right\} \leq S \left( \rho^B \right).$$

From these generalizations, we may claim that any physical admissible operation on the subsystem  $B$  of a given composite quantum system  $AB$  induced a quantum ensemble on the subsystem  $A$  for which the corresponding Holevo quantity is upper bounded by the initial von Neumann entropy of the subsystem  $B$ . We also see that in a some sense, von Neumann measurement is the most precise measurement.

**Lemma 2.5.** ([5]) A  $3 \times 3$  block matrix

$$\begin{bmatrix} A & D & E \\ D^\dagger & B & F \\ E^\dagger & F^\dagger & C \end{bmatrix}$$

defined on  $\mathbb{C}^{d_1} \oplus \mathbb{C}^{d_2} \oplus \mathbb{C}^{d_3}$  is semi-definite positive if and only if the following statements are valid:

(i)  $A \geq 0, B \geq 0, C \geq 0$ ;

(ii) there exist three contractive operators  $R_i (i = 1, 2, 3)$  such that  $D = \sqrt{A}R_1\sqrt{B}$ ,  $F = \sqrt{B}R_2\sqrt{C}$ , and

$$E = \sqrt{A}R_1\text{supp}(B)R_2\sqrt{C} + \sqrt{A - \sqrt{A}R_1\text{supp}(B)R_1^\dagger\sqrt{A}}R_3\sqrt{C - \sqrt{C}R_2^\dagger\text{supp}(B)R_2^\dagger\sqrt{C}}.$$

**Remark 2.6.** The conditions of fixed sign for the operator matrices acting on a product of Hilbert spaces play a significant role in operator theory and its numerous applications. The base result is the positivity of  $2 \times 2$  operator matrix. In [7], I. Orlov *et al.* obtained a complete description of positive definite and nonnegative operator matrices, including the suitable explicit conditions for  $3 \times 3$  operator matrices.

**Lemma 2.7.** Assume that  $U, V, W \in L(\mathbb{C}^d)$  are unitary operators and  $\mathbb{1}_d$  is the identity operator on  $\mathbb{C}^d$ . Then a  $3 \times 3$  block matrix

$$\begin{bmatrix} \mathbb{1}_d & U & V \\ U^\dagger & \mathbb{1}_d & W \\ V^\dagger & W^\dagger & \mathbb{1}_d \end{bmatrix}$$

is semi-definite positive if and only if  $V = UW$ .

*Proof.* Taking  $D = U, E = V, F = W$  and  $A = B = C = \mathbb{1}_d$  in Lemma 2.5, we have that  $R_1 = U, R_2 = W, \text{supp}(B) = \mathbb{1}_d$  and  $R_3$  is any contractive operator. Moreover,  $V = UW$ . That is

$$\begin{bmatrix} \mathbb{1}_d & U & V \\ U^\dagger & \mathbb{1}_d & W \\ V^\dagger & W^\dagger & \mathbb{1}_d \end{bmatrix} \geq 0 \iff V = UW.$$

□

**Remark 2.8.** The alternative proof of Lemma 2.7 may be given by Theorem 3.1 in [7].

### 3 The proof of the Conjecture

The main idea of the proof is as follows: We construct a  $d \otimes 3$  bipartite state  $\rho^{AB}$  such that two marginal states are  $\rho^A = \sum_{i=1}^3 p_i \rho_i$  and  $\rho^B = C_{\sqrt{F}}(\mathcal{E}_3)$ , respectively. Then next performing some von Neumann measurement on the subsystem  $B$  gives the ensemble  $\mathcal{E}_3 = \{(p_1, \rho_2), (p_2, \rho_2), (p_3, \rho_3)\}$ . By employing Lemma 2.1, it follows that the conjecture is correct.

In what follows, the proof is presented. By Polar Decomposition, we can chose three unitary matrices such that

$$\begin{aligned} |\sqrt{\rho_2}\sqrt{\rho_1}| &= U\sqrt{\rho_2}\sqrt{\rho_1} \implies \text{Tr}(\sqrt{\rho_1}U\sqrt{\rho_2}) = \sqrt{F_{12}}, \\ |\sqrt{\rho_3}\sqrt{\rho_1}| &= V\sqrt{\rho_3}\sqrt{\rho_1} \implies \text{Tr}(\sqrt{\rho_1}V\sqrt{\rho_3}) = \sqrt{F_{13}}, \\ |\sqrt{\rho_3}\sqrt{\rho_2}| &= W\sqrt{\rho_3}\sqrt{\rho_2} \implies \text{Tr}(\sqrt{\rho_2}W\sqrt{\rho_3}) = \sqrt{F_{23}}. \end{aligned}$$

Now we impose a *constraint* that  $V = UW$  on the ensemble  $\mathcal{E}_3 = \{(p_1, \rho_2), (p_2, \rho_2), (p_3, \rho_3)\}$ . Let

$$\rho^{AB} = \begin{bmatrix} p_1\rho_1 & \sqrt{p_1p_2}\sqrt{\rho_1}U\sqrt{\rho_2} & \sqrt{p_1p_3}\sqrt{\rho_1}V\sqrt{\rho_3} \\ \sqrt{p_1p_2}\sqrt{\rho_2}U^\dagger\sqrt{\rho_1} & p_2\rho_2 & \sqrt{p_2p_3}\sqrt{\rho_2}W\sqrt{\rho_3} \\ \sqrt{p_1p_3}\sqrt{\rho_3}V^\dagger\sqrt{\rho_1} & \sqrt{p_2p_3}\sqrt{\rho_3}W^\dagger\sqrt{\rho_2} & p_3\rho_3 \end{bmatrix}.$$

Clearly,  $\rho^A = \text{Tr}_B(\rho^{AB}) = \sum_{i=1}^3 p_i \rho_i$ ,  $\rho^B = C_{\sqrt{F}}(\mathcal{E}_3)$ . It remains to show that  $\rho^{AB}$  is positive. Since  $\rho^{AB}$  can be rewritten as:

$$\rho^{AB} = \begin{bmatrix} \sqrt{p_1\rho_1} & O & O \\ O & \sqrt{p_2\rho_2} & O \\ O & O & \sqrt{p_3\rho_3} \end{bmatrix} \begin{bmatrix} \mathbb{1}_d & U & V \\ U^\dagger & \mathbb{1}_d & W \\ V^\dagger & W^\dagger & \mathbb{1}_d \end{bmatrix} \begin{bmatrix} \sqrt{p_1\rho_1} & O & O \\ O & \sqrt{p_2\rho_2} & O \\ O & O & \sqrt{p_3\rho_3} \end{bmatrix}.$$

Thus by Lemma 2.7,  $\rho^{AB} \geq 0$  follows from

$$\begin{bmatrix} \mathbb{1}_d & U & V \\ U^\dagger & \mathbb{1}_d & W \\ V^\dagger & W^\dagger & \mathbb{1}_d \end{bmatrix} \geq 0 \text{ only when } V = UW.$$

Clearly  $\dim \mathcal{H}^B = 3$ . Let  $\{|0^B\rangle, |1^B\rangle, |2^B\rangle\}$  be an orthonormal basis for  $\mathcal{H}^B$  such that  $p_j \rho_j^A = \langle j^B | \rho^{AB} | j^B \rangle$ . It follows from Lemma 2.1 that

$$\chi(\mathcal{E}_3) = \chi \left\{ (p_j, \rho_j^A) \right\} \leq S(\rho^B) = S(C_{\sqrt{F}}(\mathcal{E}_3)).$$



From the above discussion, we can have the following conclusion as a by-product in this paper:

**Proposition 3.1.** *There exists a bipartite Hermite operator, acting on a Euclidean space  $\mathbb{C}^d \otimes \mathbb{C}^3$  ( $1 < d \in \mathbb{N}$ ), which is not positive semi-definite, but whose two marginals are positive semi-definite.*

It is *conjectured* that for any  $1 < d_1, d_2 \in \mathbb{N}$ , there exists a bipartite Hermite operator, acting on a Euclidean space  $\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2}$ , which is not positive semi-definite, but whose two marginals are positive semi-definite.

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## 4 Appendix

In this section, we develop an interesting characterization of positivity for a special block matrix with each entry being a  $d \times d$  unitary matrix. The proof can be easily derived from the main result in [7], so it is omitted here.

Assume that a collection  $\mathbf{U}$  of unitary operators  $\{U_{ij} : i, j = 1, \dots, K\}$  such that  $K \times K$  operator matrix

$$\begin{bmatrix} U_{11} & U_{12} & \cdots & U_{1K} \\ U_{21} & U_{22} & \cdots & U_{2K} \\ \vdots & \vdots & \ddots & \vdots \\ U_{K1} & U_{K2} & \cdots & U_{KK} \end{bmatrix}$$

is positive semi-definite. Then these unitary operators in  $\mathbf{U}$  satisfy the conditions:

- (i)  $U_{ii} = \mathbb{1}_d$  for each index  $i$ ;
- (ii)  $U_{ji} = U_{ij}^\dagger$  for all indices  $i, j$ ,

Clearly, if  $U_{ij} = U_i U_j^\dagger$ , where  $\{U_i : i = 1, \dots, K\}$  consists of  $K$  unitary operators, then  $[U_{ij}]$  is positive semi-definite.

**Theorem 4.1.** Assume that  $\{U_{ij} : i, j = 1, \dots, K\}$  is a collection of  $d \times d$  unitary matrices. Let  $P = [U_{ij}]$ . If  $P \geq 0$ , then the following statements are equivalent:

1.

$$P = \begin{bmatrix} \mathbb{1}_d & U_{12} & \cdots & U_{1K} \\ U_{12}^\dagger & \mathbb{1}_d & \cdots & U_{2K} \\ \vdots & \vdots & \ddots & \vdots \\ U_{1K}^\dagger & U_{2K}^\dagger & \cdots & \mathbb{1}_d \end{bmatrix} \geq 0.$$

2.

$$P = \begin{bmatrix} \mathbb{1}_d & U_1 & U_1 U_2 & U_1 U_2 U_3 & \cdots & \cdots & U_1 U_2 \cdots U_{K-1} \\ U_1^\dagger & \mathbb{1}_d & U_2 & U_2 U_3 & U_2 U_3 U_4 & \ddots & \vdots \\ U_2^\dagger U_1^\dagger & U_2^\dagger & \mathbb{1}_d & U_3 & U_3 U_4 & \ddots & \vdots \\ U_3^\dagger U_2^\dagger U_1^\dagger & U_3^\dagger U_2^\dagger & U_3^\dagger & \mathbb{1}_d & \ddots & \ddots & U_{K-3} U_{K-2} U_{K-1} \\ \vdots & \ddots & \ddots & \cdots & \ddots & \ddots & U_{K-2} U_{K-1} \\ \vdots & \ddots & \ddots & \cdots & \ddots & \ddots & U_{K-1} \\ U_{K-1}^\dagger \cdots U_2^\dagger U_1^\dagger & \cdots & \cdots & U_{K-1}^\dagger U_{K-2}^\dagger U_{K-3}^\dagger & U_{K-1}^\dagger U_{K-2}^\dagger & U_{K-1}^\dagger & \mathbb{1}_d \end{bmatrix}$$

for a collection  $\{U_i : i = 1, \dots, K-1\}$  of  $d \times d$  unitary operators.

3.

$$P = \begin{bmatrix} V_1 \\ V_2 \\ \vdots \\ V_K \end{bmatrix} \begin{bmatrix} V_1^\dagger & V_2^\dagger & \cdots & V_K^\dagger \end{bmatrix}$$

for a collection  $\{V_i : i = 1, \dots, K\}$  of  $d \times d$  unitary operators.

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